Sources of Evaluated Data

All subshell parameters are theoretical as opposed to experimental. The basic subshell data and the radiative widths came from the work of J. H. Scofield[6-9]. The nonradiative widths came from the results of M. H. Chen[10-16]. The transition probabilities were evaluated as described in the section,Transition Probabilities and Widths.

Procedures Used to Derive Data

Assumptions and Approximations

This library contains data for subshells that are occupied when an atom is in its neutral, ground state. Data are not included for initially ionized or excited atoms.

The library does not describe the electron that is emitted when the atom is initially ionized. It is assumed that this electron has been explicitly accounted for based on the kinematics of the ionizing event, e.g., photoelectric, electron impact ionization, or internal conversion. It is also assumed that once ionized, the relaxation is independent of how the atom was initially ionized.

The relaxation data in the library is designed to describe the bound-bound radiative and nonradiative transitions following an ionization event. Additionally it is assumed that relaxation only occurs where both radiative and nonradiative transitions are possible.

It is also assumed that the binding energy of all subshells are the same for neutral ground state atoms as for ionized atoms. This assumption has been adopted because at the current time there is no provision to provide complete data describing the binding energy of each subshell of an atom when any of its other subshells is singly or multiply ionized.

Subshell data are provided for Z = 1 through 100; however, transition probabilities are only explicitly included for Z = 6 through 100. Therefore, for Z = 1 through 5 the library only includes a local energy deposit corresponding to the binding energy of an electron in each subshell.

Relaxation data is provided for all subshells that are occupied when an atom is in its neutral ground state. However, transition probabilities are only explicitly included for most subshells. For the outer subshells, the radiative transition probability is very small. Also, the binding energy of an electron is very small so that radiative or nonradiative transitions will lead to the emission of very low energy photons or electrons. In either case these may be considered to deposit their energy locally. Therefore for the outer subshells, the library only includes a local energy deposit corresponding to the binding energy of an electron in each subshell.

Transition Probabilities and Widths

The creation of a vacancy in an atomic subshell initiates a series of complex transitions as the vacancy moves to outer subshells and the atom relaxes back to the stable configuration. There are two types of transitions, radiative and nonradiative. In a radiative transition, a vacancy in one subshell is filled by an electron from an outer subshell with the release of fluorescence radiation, i.e., x-ray emission. In a nonradiative transition, the initial vacancy is filled by an electron from an outer subshell, the available energy given to the removal of an electron from the same subshell or from one further out. This process results in two electron